SuperMIC supercomputer to impact research nationally

Imagine having to test thousands of complex molecular interactions to develop the perfect targeted drug. On a regular computer, this would be an impossible task due to the simultaneous movements and relationships of each and every atom. Louisiana academic researchers will soon have the ability to quickly perform these complicated calculations on SuperMIC, a new supercomputer that will have a processing speed of over a quadrillion calculations per second.

Built with tens of thousands of computer processing cores and hundreds of accelerated coprocessors and immense memory, the new supercomputer will be able to process complex molecular visualizations and calculations quickly and efficiently.

With a debut processing speed exceeding 10^{15} floating-point operations per second (1 PFLOPS), SuperMIC will be one of the fastest academic supercomputers in the United States.

SuperMIC will be ideal for leveraging existing resources and extending large, multi-disciplinary projects, like forecasting hurricane storm surges, biomolecular transportation and drug delivery, and accelerated development of advanced manufacturing for new materials.

Academic and private sector partnerships will be further facilitated with this opportunity to take advantage of SuperMIC's computing capabilities to speed up research and development and hasten delivery to the market, such as modeling chemical reactions to develop the next generation of batteries. In addition, the computer cluster will be an asset to Louisiana's booming entertainment industry as a resource for digital media projects.

SuperMIC will be purchased with a $4 million Major Research Instrumentation Program grant from the National Science Foundation awarded to the Center for Computation & Technology (CCT), and will be housed in the Frey Computing Services Center at Louisiana State University.

The supercomputer project is led by Dr. Honggao Liu, Deputy Director of CCT, and co-investigators Joel Tohline, Qin Chen, Jagannathan
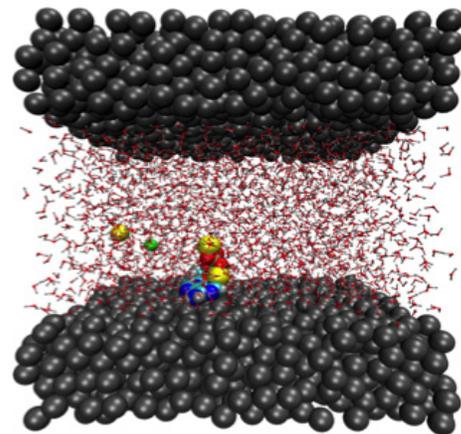
Graphic vizualization of the transport of a bio-molecule in an aqueous environment. Source: Louisiana Alliance for Simulation-Guided Materials Applications professors Dimitris Nikitopoulos and Dorel Moldovan.

Ramanujam and Mark Jarrell.

In addition to the immense computing power and time savings, SuperMIC will link Louisiana universities via the Louisiana Optical Network Initiative (LONI) which supports 20 universities, two medical schools, three partner organizations and over 70 community and technical colleges. The network is evolving and will soon operate at 100 Gbps.

SuperMIC will also be an asset to the national research community, as it will be linked to the national

"SuperMIC is an integral part of Louisiana cyberinfrastructure and will contribute to big data research in the state. Louisiana researchers will use SuperMIC to provide solutions across a spectrum of challenges, such as providing medical data integration, improving disease identification, addressing health disparities and personalized medicine, improving extraction of Earth-based energy resources, facilitating the smart energy grid, accelerating materials development, and improving the prediction of hurricanes and coastal erosion."

- Dr. Honggao Liu, Deputy Director, Louisiana State University, Center for Computation & Technology

supercomputer infrastructure network which connects 16 supercomputers and high-end visualization and data analysis resources.

Forty percent of the usage of Super-MIC will be utilized by the National Science Foundation's Extreme Science and Engineering Discovery Environment (XSEDE), the most advanced and powerful collection of integrated advanced digital resources and services in the world.

"I look forward to connecting Super-MIC to Louisiana's optical network and the national infrastructure because it will enable science discovery and to solve large, complicated problems in the world," said Dr. Honggao Liu, Deputy Director of CCT.

Dr. Honggao Liu

The interactions this project will bring will greatly benefit Louisiana researchers in diverse disciplines. For example, the materials scientists partnered in the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA) are exploring a wide technologies ranging from new materials to targeted medicines. "However, they all have overlapping sets of mathematical equations that the supercomputer will be taught to solve effectively. Working interactively will help spur innovation and everyone will benefit from this collaboration," said Dr. Michael Khonsari, State of Louisiana Associate Commissioner for Sponsored Programs Research and Development.

A critical part of the supercomputer program will be training students to use the new architecture. These skills will be integral to programming the smart phones and computers of the future.

"We need to start by teaching young girls and boys basic computer knowledge starting with tangible devices like laptops, tablets or mobile devices. Today's mobile phones are more powerful than the fastest supercomputer in the world 25 years ago. The power of the number one supercomputer today could be held in the new smartphone 20 years from now," said Liu.
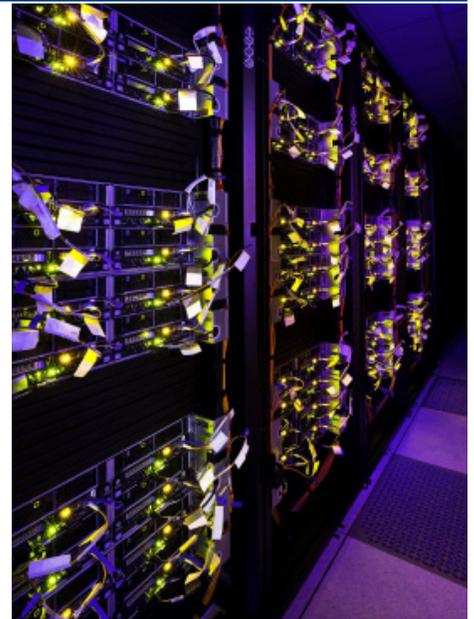
Supercomputer racks bathed in purple and gold light, John Livzey, LSU.

One such program, called "Alice in Computerland," teaches 6-8th grade girls how to build a website or make a movie to help them develop an interest in computers. Later, the students are introduced to programming and high performance computing.

Training and education will be provided to older students across the state as well, through distance learning classes and hands-on workshops held in conjunction with LONI and LA-SiGMA.